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Kampus Sungai Petani

Faculty of Administrative
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PREDICTION OF NANOSTRUCTURE OF SnO₂ PROPERTIES USING ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

Tin(IV) oxide, SnO₂ nanostructures such as nanorods, nanoflowers, nanosheets, nanocubes have been receiving significant interest in various fields due to their inherent properties. The types of shape and size of nanorods vary based on the applications. A fine tuning of the parameters (e.g concentration, pH, temperature, template, type of solvent etc.) during the synthesis process can alter the morphology of the SnO₂. However, producing nanostructures with the desired size and shape is extremely complex and still remains a challenge. Hence, in this study a mathematics modelling called Artificial Neural Network (ANN) for the prediction of the SnO₂ morphology was developed. This study was carried out using the real time data collected *via* experimental work and training the data using a neural network toolbox in MATLAB Version (R2016a) software. An ANN modelling was constructed with the input parameters of reaction time and concentration of precursors and three different output parameters namely, crystalline size, band gap energy and size of particles. This modelling was developed based on trial and error at different network architecture, activation function and training algorithm. The data set was trained using hyperbolic tangent sigmoid (tansig) activation function and Levenberg-Marquardt training algorithm. The performance of modelling was evaluated based on the mean square error (MSE) and coefficient of determination (R²). The finding shows, there is no overfitting while constructing the neural network and it is able to track the data. The result shows that the MSE performance plot and R² are in the range of 0.1-1.0. Therefore, it is suggested that the ANN modellings constructed in this study are able to produce a decent prediction. These values indicate that prediction of nanostructure SnO₂ properties using artificial neural network (ANN) is a great success.

Keywords: SnO₂, nanostructures, ANN, process modelling, hyperbolic tangent sigmoid, Levenberg-Marquardt training

INTRODUCTION

Tin (IV) oxide nanostructures represent an important class of crystalline semiconducting nanomaterial as it shows exceptional characteristics for instance high surface to volume ratio, high electron mobility ($100\text{-}200\text{ cm}^2\text{ V}^{-1}\text{ S}^{-1}$) (Inderan et al, 2015), large energy gap (3.1-3.6eV) (Karmaoui et al, 2018), low electrical resistivity, high optical transparency and high theoretical specific capacity which made it one of the most popular metal oxide nanostructures. Several techniques have been developed for the preparation of SnO₂ nanostructures such as hydrothermal, sol-gel, wet chemical synthesis, co-precipitation, etc (Dontsova et al, 2017). Among them, the hydrothermal method has been extensively used to synthesize SnO₂ nanostructures due to its high efficiency, simplicity and economical fabrication (Kundu et al, 2019). In addition, hydrothermal synthesis can generate nanomaterials that are stable at elevated temperatures, and by liquid phase or multiphase chemical reactions, the composition of nanomaterials to be synthesized can be well regulated. Nanomaterials with high vapor pressure can also be generated with minimal loss of materials by this process (Gan et al, 2020).

The properties of nanostructures of SnO₂ can be simply tuned by changing the experimental parameters such as concentration, pH, temperature, template, solvent form, etc. However, to obtain a nanostructure with a desired size and shape remains a challenge. Therefore, Artificial Neural Network (ANN), a mathematical modelling can ease the process for the prediction of SnO₂ nanostructure properties. To create an optimal ANN model, there are few significant parameters to consider, namely the number of neurons in input, output and hidden layers. To build a successful network, the number of hidden layers, weights, bias, activation function and training algorithm must also be considered as ANN model for this research consists of several neurons. First, input neurons received input parameters fed into the network and stored the scale of the value input and calculated the value of the output layer called as output neuron. Hidden layers are located between the layers of input and output and are linked to each other. The sum of input and output values in each neuron will be weighted and added with a parameter called bias and the sum is passed through a function called the activation function. This activation function produces an output by taking into consideration all the contributions from its input links. Therefore, this study emphasizes on the prediction of the nanostructure SnO₂ properties synthesized at different reaction time and concentration of metal precursors *via* hydrothermal method. The particle size, band gap energy and crystalline size are selected as SnO₂ important properties in order to create the ANN models.

METHODOLOGY

The data were obtained from the analysis of nanostructure of SnO₂ that was conducted experimentally (Inderan et al, 2015). Two different experimental works have been carried out. The first experimental work was performed at a relatively low temperature (180 °C) and at pH 13 using different reaction times (6 hours, 12 hours, 18 hours and 24 hours). The second experimental work was carried out at the same temperature using various concentration of metal precursors (0.04M, 0.08M, 0.12M, 0.16M and 0.20M) in a mixed solution of water and ethanol by adding 6M NaOH to obtain the desired pH, pH 13.

Depending on the data collection, the hidden layer arrangement of this ANN model can be built either in multi-layer or single layer. In this analysis, the input dataset is divided into three sets, 70% of the data collection are for the training of data, 15% of the data is considered validation data, and the remainder 15% of the data is assigned for test data. Back propagation (BP) feed

forward neural network is employed because it is possible to adjust the number of hidden layers and neurons in each hidden layer according to any circumstances. The Levenberg-Marquardt (trainlm) algorithm is used in a typical BP neural network. The transfer function that is chosen is tangent sigmoidal (tansig). The trial and error of the number of hidden neurons will be a good strategy for this neural network model to get the optimal results. ANN model will be constructed where the input parameters are time and concentration of precursors while the output parameters are band gap energy of the metal oxide SnO₂, diameter of the particle size and lastly, crystalline size.

RESULT AND DISCUSSION

Figure 1 demonstrates the neural network design for the prediction of nanostructure of SnO₂ properties that consist of two input layers, a hidden layer and three output layers. Performance of the neural network design can be evaluated based on mean square error (MSE) and R², a coefficient of determination. Figure 2(a) presents the result of R² which is also referred to as “goodness of fit” as it measures how strong the linear relationship is between the two variables and gives a value of 0.99895. The value of MSE that is shown in Figure 2(b) gives a value of 0.12748 where it falls in the range of 0.1-1.0 which means that it is a highly reliable prediction model. Table 1 tabulates various values of mean square error (MSE) and regressions for the network designed during training, validation and testing process.

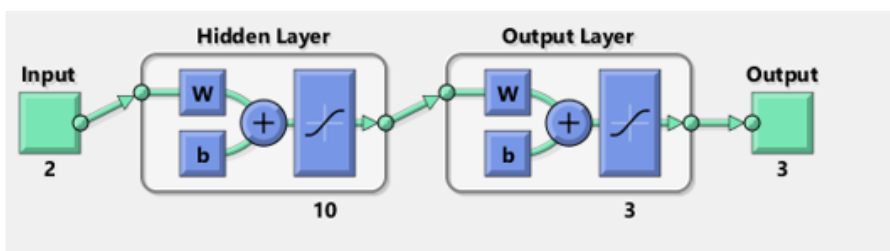


Figure 1: Neural network design for the prediction of properties of SnO₂

Table 1: Mean square error (MSE) and regression for network design

Fitting Network Sequence	Setup Division of Data	Performance (MSE)			Regression		
		Training	Validation	Testing	Training	Validation	Testing
2-10-3	70-15-15	0.3147	0.12748	0.3791	0.99868	1	0.99999

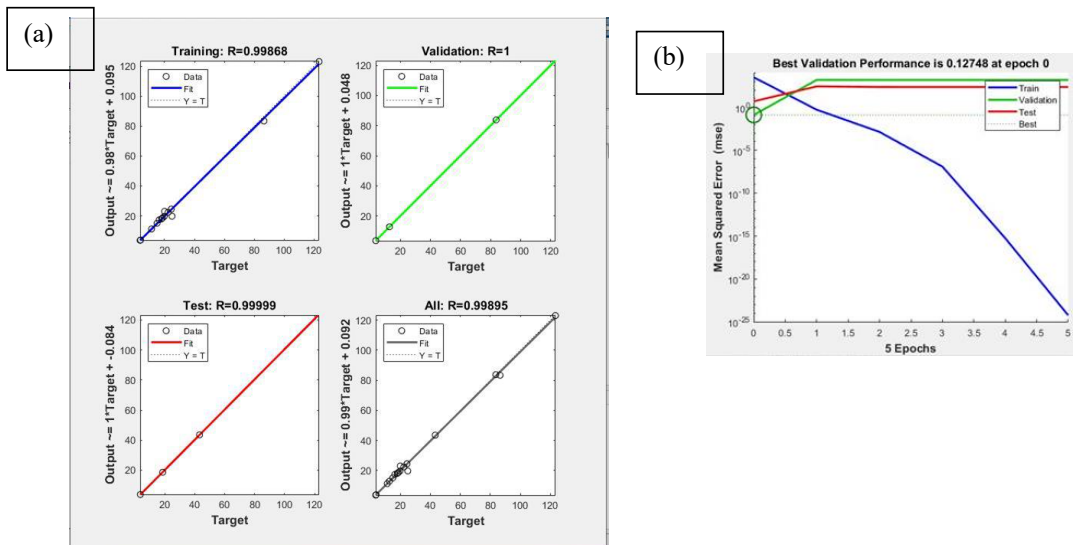


Figure 2 : (a) Neural network regression and (b) Validation performance for ANN model

An ANN model was successfully developed to predict the properties of SnO₂ nanostructures in which the accuracy of the model is highly dependent on the training data. Hence, in order to produce a highly reliable model that is accurate, an excellent collection of training data is required. The data presented should be well distributed, sufficient and measured accurately. Although the data are small, the results generated are properly trained and give an excellent result.

CONCLUSIONS

The prediction of properties of nanostructure of SnO₂ using ANN was successfully achieved. The network uses two different inputs namely reaction time and concentration of precursor with a neural network topology of 2-10-1. The values of R^2 ranging from 0.95-1.0 show that there is a high correlation of experimental data and predicted results proving a correct evaluation with the least error. As a conclusion, this research shows that an intelligent system such as ANN is able to develop a neural network model precisely as the best alternative compared to the conventional method as it produces an acceptable accuracy.

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